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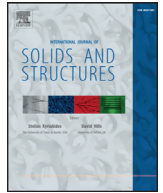
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How strong is the temperature increase due to a moving dislocation?



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ABSTRACT

This article calculates the temperature increase resulting from the motion of a dislocation. The temperature rise is ascribed to two separate effects, both of which are calculated: the dissipative effect resulting from the energy lost by the dislocation as it overcomes the intrinsic lattice resistance to its motion; and the thermomechanical effect arising from the constrained changes in volume the dilatational field of a moving dislocation may entail. The dissipative effect is studied in an uncoupled continuum solid, whilst the thermomechanical effect is studied in a fully coupled thermo-elastodynamic continuum. Explicit solutions are provided, as well as asymptotic estimates of the temperature field in the immediacy of the dislocation core.

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1. Introduction

Fast moving dislocations are usually associated with an increase in the temperature of the surrounding medium because the motion of a dislocation is overdamped (Hirth and Lothe, 1982): a dislocation will not move unless an external stimulus is applied to it, and any energy spent in moving a dislocation will eventually be dissipated as heat (Eshelby and Pratt, 1956). The energy required to move a dislocation increases with its speed (Weertman, 1961); but, at the same time, the ability of the medium to dissipate heat away from the dislocation's core is limited by its thermal conductivity. Thus, one ought to expect increased localised heating around the dislocation as its moves with increasing speeds.

In addition to this 'dissipative' heating effect, edge dislocations carry a dilatational¹ field about their core. Since constrained changes in volume are associated with an increase in temperature (Callen, 1985), one ought to expect an increase in temperature associated with the dilatational field of the dislocation. This temperature increase would be caused by thermomechanical effects alone (see Chadwick, 1960; Nowacki, 1962), which are separate from (albeit sometimes accounted for by) the dissipative heating described above, but that could prove to be equally relevant for high speed dislocations, because an edge dislocation's dilatational fields are known to contract and magnify with increasing speed (see Gurrutxaga-Lerma et al., 2013). Because of their inherent cylindrical symmetry, the stress tensor of a screw dislocations

is traceless, so unlike the dissipative effect, the thermomechanical heating effect can only be associated with edge dislocations.

Based on the asymptotic behaviour of the stationary temperature field radiated by a steady point source in a cylinder, Eshelby and Pratt (1956) suggested that a distribution of moving dislocations could explain localised thermal stresses leading to microcracks. Similar models were subsequently used to argue that, for instance, adiabatic shear band formation could be explained by an avalanche of dislocations suddenly released from a pile-up (Armstrong et al., 1982; Armstrong and Elban, 1989). De Hosson et al. (2001), employing arguments in line with Eshelby and Pratt's, went further to produce a numerical model that coupled the total energy radiated by a planar distribution of dislocation with Fourier's law applied in a periodic planar system constricted by adiabatic walls. Their model suggested that the heating resulting from moving dislocations could be considerable, and associated the latter with the appearance of thermomechanical effects affecting the plastic deformation of the solid. Brock (1992) employed a coupled thermomechanical model of a crack with an injected dislocation to determine the temperature rise around a loaded crack tip. Experimental studies have associated such effects with plastic deformation (Ravichandran et al., 2001), adiabatic shear band formation (Armstrong and Zerilli, 1994; Zhou et al., 1996; Guduru et al., 2001), flash heating in earthquakes (Spagnuolo et al., 2016), and microcrack formation under fatigue loading (Dowling and Begley, 1976; Guo et al., 2015), amongst many others. Thus, the temperature increases resulting from the activity of fast moving dislocations appears to have a definite impact in the local temperature distribution in a crystalline solid and in its mechanical response.

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¹ Equivalent to a hydrostatic or pressure field.

The aim of this article is to study the localised increase in temperature that may be induced by a moving dislocation in a crystalline medium, developing models able to estimate the transient heating effects induced by a dislocation in its motion. To this end, Section 2 introduces an analytical model to estimate, on energetic grounds alone, the dissipative temperature increase by a moving dislocation modelled as a point heat source. Since the point source model neglects thermomechanical transport, Section 3 will be devoted to the thermomechanical dislocation, deriving the field equations for a dislocation moving in a dynamic thermomechanical medium; these solutions will be approximated in Section 4. Finally, Section 5 will summarise the main findings of this article.

2. Analytical estimates of the dissipative temperature increase induced by a moving dislocation

The simplest way to study the temperature increase induced by a moving dislocation is to revisit Eshelby and Pratt's suggestion that all the work exerted to make a dislocation move must eventually be dissipated as heat (Eshelby and Pratt, 1956).

The value of the physical constants involved is assumed to remain independent of temperature; as will be seen, this is a reasonable approximation. In that case, an infinite straight dislocation of either edge or screw character can be modelled as a heat source moving in a planar medium, in which case the temperature field will be governed by Fourier's law:

$$K\nabla^2\theta(x, y, t) = \rho c_v \dot{\theta}(x, y, t) - q_v(x, y, t) \quad (1)$$

where hereafter $\theta = T - T_0$ is the temperature field relative to some reference value T_0 , K the thermal conductivity, ρ the material's density, c_v the specific heat at constant deformation, and $q_v(x, y, t)$ a heat source term.

Although the dislocation will have some spatial width (Hirth and Lothe, 1982), it can be modelled as a point heat source. In the following, the dislocation will be gliding along the x axis with speed v . As said, the motion of a dislocation is overdamped, any work exerted to move it will eventually be released and dissipated in the form of heat. Thus, one may estimate the heat radiated by the dislocation in terms of the work exerted to move the dislocation (see Eshelby and Pratt, 1956):

$$q_v = B\tau v \delta(x - vt) \delta(y) \quad (2)$$

where τ is the resolved shear stress applied over the dislocation, B the magnitude of the Burgers vector, and v the dislocation's glide speed; the $\delta(x - vt)\delta(y)$ factor accounts for the fact that the heat source moves along the x axis, and is concentrated on the $y = 0$ plane.

The glide speed v is related to the resolved shear stress τ via the dislocation's mobility law. Generally, the mobility law may be written as

$$\tau = \tau(v) \quad (3)$$

where $\tau(v)$ appropriately captures the different microscopic dissipative effects (phonon wind Nabarro, 1967; De Hosson et al., 2001, phonon scattering Hirth and Lothe, 1982, radiative damping Pellegrini, 2014, etc.) that contribute to the crystalline lattice's intrinsic resistance to the motion of the dislocation. The specific form of the mobility law is a matter of choice; here the main requirement is that for low speeds the slope of $\tau(v)$ matches the observed linear viscous drag coefficient (see Hirth and Lothe, 1982), and that it saturates as the speed approaches the transverse speed. Here, as a first approach one can assume a relationship of the following kind (Gurrutxaga-Lerma, 2016):

$$B\tau = v \frac{d_0}{1 - \frac{v^2}{c_t^2}} \quad (4)$$

where d_0 is the low speed drag coefficient, and c_t the transverse speed of sound. This mobility law accounts, phenomenologically, for the relativistic effects that drive the dislocation's elastic (and kinetic) energy towards infinity as its speed approaches the transverse speed of sound, c_t .

This enables the writing of Eq. (1) as

$$\kappa_v \nabla^2 \theta = \dot{\theta} + q \delta(x - vt) \delta(y) \quad (5)$$

where $\kappa_v = K/(\rho c_v)$ is the material's thermal diffusivity at constant deformation, and where $q = \frac{1}{\rho c_v} \frac{v^2 d_0}{1 - \frac{v^2}{c_t^2}}$ is the source's energy release rate.

For simplicity, assume that v is independent of t (i.e., that the applied resolved shear stress τ is kept constant throughout the motion of the source). In that case, the problem is reduced to that of a moving heat source that releases energy at a constant rate q . As an initial condition, it is assumed that at $t = 0$ the temperature of the system is undisturbed, i.e., $\theta(x, y, 0) = 0$. The solution to this problem is derived in the following.

Define the following Fourier transform for the two spatial variables x and y :

$$\Theta(\underline{k}, t) = \int_{\mathbb{R} \times \mathbb{R}} \theta(\underline{r}, t) e^{i \underline{k} \underline{r}} d\underline{r} \quad (6)$$

where $\underline{k} = (k_x, k_y)^T$ and $\underline{r} = (x, y)^T$.

Applying it to Eq. (5)

$$\kappa_v \Theta |\underline{k}|^2 = \frac{\partial \Theta}{\partial t} - Q(\underline{k}, t) \quad (7)$$

where

$$Q(\underline{k}, t) = \int_{\mathbb{R} \times \mathbb{R}} q \cdot \delta(x - vt) \delta(y) e^{i(k_x x + k_y y)} dx dy = q e^{i k_x vt} \quad (8)$$

The solution to the equation provided that initially $\theta(x, y, 0) = 0$ throughout the infinite domain, will be (Hobson et al., 2006)

$$\Theta(\underline{k}, t) = \int_0^t e^{-\kappa_v |\underline{k}|^2 (t-t')} Q(\underline{k}, t') dt' \quad (9)$$

For later convenience, call:

$$G(\underline{k}, t, t') = e^{-\kappa_v |\underline{k}|^2 (t-t')}, \quad (10)$$

The inverse Fourier transform will be

$$\begin{aligned} \theta(x, y, t) &= \frac{1}{2\pi} \int_{\mathbb{R} \times \mathbb{R}} \Theta(\underline{k}, t') e^{-i \underline{k} \underline{r}} d\underline{k} \\ &= \frac{1}{2\pi} \int_0^t dt' \int_{\mathbb{R} \times \mathbb{R}} d\underline{k} G(\underline{k}, t, t') Q(\underline{k}, t') e^{-i \underline{k} \underline{r}} d\underline{k} \end{aligned} \quad (11)$$

Invoking the convolution theorem for Fourier transforms,

$$\int_{\mathbb{R} \times \mathbb{R}} G(\underline{k}, t, t') \cdot Q(\underline{k}, t, t') e^{i \underline{k} \underline{r}} d\underline{k} = \int_{\mathbb{R} \times \mathbb{R}} g(\underline{r} - \underline{r}', t) q(\underline{r}', t) d\underline{r}' \quad (12)$$

it follows that

$$\theta(x, y, t) = \frac{1}{2\pi} \int_0^t dt' \int_{\mathbb{R}} g(\underline{r} - \underline{r}', t, t') q(\underline{r}', t, t') d\underline{r}', \quad (13)$$

where the inverse Fourier transform of the function G is in fact known:

$$g(\underline{r}, t, t') = \frac{1}{2\pi} \int_{\mathbb{R} \times \mathbb{R}} e^{-\kappa_v |\underline{k}|^2 (t-t')} e^{-i \underline{k} \underline{r}} d\underline{k} = \frac{1}{2\kappa_v (t-t')} e^{-\frac{|\underline{r}|^2}{4\kappa_v (t-t')}} \quad (14)$$

From this, it immediately follows that

$$\theta(x, y, t) = \frac{1}{2\pi} \int_0^t \frac{1}{2\kappa_v (t-t')} \int_{\mathbb{R} \times \mathbb{R}} e^{-\frac{(x-x')^2 + (y-y')^2}{4\kappa_v (t-t')}} q \delta(x' - vt) \delta(y') d\underline{r}' \quad (15)$$

Resolving the spatial integral is immediate, and substituting the value of q , one finally obtains:

$$\theta(x, y, t) = \frac{1}{4\pi K} \frac{v^2 d_0}{1 - \frac{v^2}{c_t^2}} \int_0^t \frac{e^{-\frac{(x-vt')^2 + y^2}{4\kappa_v(t-t')}}}{t-t'} dt', \quad (16)$$

which provides a simple estimate of the temperature field surrounding a dislocation moving with uniform speed v .

This procedure could also be used to derive a more general expression relevant for the case in which the dislocation moves non-uniformly with speed $v = v(t)$. In that case, one would find that²

$$\theta(x, y, t) = \frac{1}{4\pi K} \int_0^t \frac{v^2(t') d_0}{1 - \frac{v(t')^2}{c_t^2}} \frac{e^{-\frac{(x-v(t')t')^2 + y^2}{4\kappa_v(t-t')}}}{t-t'} dt', \quad (18)$$

Eq. (16) describes the temperature field around the dislocation in terms of a quasi-exponential integral function (cf. Gradshteyn and Ryzhik, 2007), which is easily solved numerically. It also allows for a number of asymptotic expressions outlined in the following. For values of x close to the core's position at vt , the integral in Eq. (16) may be asymptotically approximated to first order³ as:

$$\theta(x, y, t) \approx \frac{1}{4\pi K} \frac{v^2 d_0}{1 - \frac{v^2}{c_t^2}} \int_0^t \frac{e^{-\frac{y^2}{4\kappa_v(t-t')}}}{t-t'} dt', \quad (19)$$

which entails that about the dislocation's core and in the direction of slip ($y = 0$), the dissipative temperature field ought to scale with the prefactor alone, i.e., that the dependence of the temperature field around a dislocation's core with respect to the dislocation's speed is, to a good approximation, of the form

$$\theta(v) \approx \frac{1}{4\pi K} \frac{v^2 d_0}{1 - \frac{v^2}{c_t^2}} \quad (20)$$

For $v = 0.99c_t$, using the material properties of FCC aluminium, $\theta(v)$ has a magnitude of $\approx 15\text{K}$; for $v = 0.01c_t$, it has gone down to 10^{-5}K . One should expect that a dislocation moving at speeds close to the shear wave speed would heat up the surrounding material with an intensity about 5 order of magnitudes higher than at low speeds. The evolution of Eq. (20) with increasing v is depicted in Fig. 2.

This is confirmed in Fig. 1, which shows the temperature distributions arising from Eq. (16) for dislocations moving at different speeds. As can be seen, at a distance roughly $\approx 0.5\mu\text{m}$ away from the dislocation core, the temperature increase this model entails ranges from 10^{-5}K at $v = 0.01c_t$ (Fig. 1a) through to 10^{-1}K at $v = 0.66c_t$ (Fig. 1c) all the way up to temperature increases in excess of 5K for dislocations moving with $v = 0.99c_t$ (Fig. 1d).

More generally, one may expand Eq. (16) in series of v about 0, in which case,

$$\theta(x, y, t) \approx \frac{1}{4\pi K} \frac{v^2 d_0}{1 - \frac{v^2}{c_t^2}} \int_0^t \frac{e^{-\frac{x^2 + y^2}{4\kappa_v(t-t')}}}{t-t'} dt', \quad (21)$$

The integral is a pure exponential integral function. For values of $r = \sqrt{x^2 + y^2}$ very close to the dislocation core (i.e., $r \rightarrow 0$), the asymptotic behaviour of the exponential integral is dominated by

² More generally, for any one form of q such that $q(t)$ is integrable and spatially localised in the bulk (i.e., not a boundary), Eq. (15) may be written as

$$\theta(x, y, t) = \frac{1}{4\pi K} \int_0^t q(t') \frac{e^{-\frac{(x-v(t')t')^2 + y^2}{4\kappa_v(t-t')}}}{t-t'} dt', \quad (17)$$

which holds for any one $q = B\tau v$ so long as these variables are integrable.

³ By expanding the integrand in Taylor series of v about x/t .

$\ln(r^2/(4t\kappa_v))$ (see Gradshteyn and Ryzhik, 2007), so that

$$\theta(x, y, t) \approx \frac{1}{4\pi K} \frac{v^2 d_0}{1 - \frac{v^2}{c_t^2}} \ln\left(\frac{x^2 + y^2}{4\kappa_v t}\right) \quad (22)$$

which, excluding dimensionality,⁴ may be compared to the asymptotic expression achieved by Eshelby and Pratt (1956) when $t = r/v$ for the quasi-stationary case:

$$\theta(x, y, t) \approx \frac{1}{2\pi K} \frac{v^2 d_0}{1 - \frac{v^2}{c_t^2}} \ln\left(\frac{v\sqrt{x^2 + y^2}}{2\kappa_v}\right) \quad (23)$$

The energy dissipated in this way by a single dislocation will be superimposed to that of others; for dense distributions of fast moving dislocations such as those that may be encountered at high strain rates, the increase in temperature can therefore be substantial. Still, the temperature increase predicted by this simple model is modest enough to justify the constant value of the material constants in this analysis, as well as the invariance with temperature of the dislocation's phonon drag coefficient (here, d_0).

The model above is fully uncoupled from the elastic fields of the dislocation; however, increased temperature ought to entail the appearance of thermal stresses about the dislocation core and, vice versa, the mechanical fields of the dislocation ought to entail changes in the temperature about the core. In fact, since the primary mode of energy radiation away from the core is through elastic waves (acoustic phonons) (Pellegrini, 2014), it seems necessary to modify the account given above to relate the increase in temperature driven by the dislocation with the thermal stresses these may produce. This is done in the following section.

3. Thermomechanical effects on dislocation motion

In thermodynamical systems, constrained changes of volume entail variations of temperature, and vice versa (Callen, 1985). The elastic field of an edge dislocation carries a hydrostatic component around the dislocation's core (Hirth and Lothe, 1982), so it is to be expected that the dislocation will act as a source of thermal stress. Since the moving dislocation is known to experience contractions as it speeds up towards the transverse speed of sound (Gurrutxaga-Lerma et al., 2014), the thermal distribution and thermomechanical effects surrounding the dislocation core are expected to be modified. Here the way in which this process happens is explored.

3.1. Governing equations of the dynamic thermoelastic problem

The way temperature affects volumetric changes may be expressed via following eigenstrain (cf. Mura, 1982):

$$\epsilon_{ij}^* = \alpha_L (T - T_0) \delta_{ij} \quad (24)$$

where α_L is the linear thermal expansion coefficient, T_0 some reference temperature, and ϵ_{ij}^* denotes the first order strain tensor. This eigenstrain associates a dilatational strain with a change of temperature from a reference value T_0 ; as a first approach approximation, the dilatation strain is made to be linearly dependent with temperature. As in Section 2 for brevity, hereafter

$$\theta \equiv T - T_0 \quad (25)$$

The eigenstrain will modify the general elastic strain tensor as $\epsilon_{ij} - \epsilon_{ij}^*$ (see Mura, 1982). Accordingly, Hooke's law for a linear isotropic solid is modified into (Chadwick, 1960)

$$\sigma_{ij} = \Lambda \epsilon_{kk} \delta_{ij} + 2\mu \epsilon_{ij} - \alpha_L (3\Lambda + 2\mu) \theta \delta_{ij} \quad (26)$$

⁴ The solution employed by Eshelby and Pratt applies to axisymmetric systems.

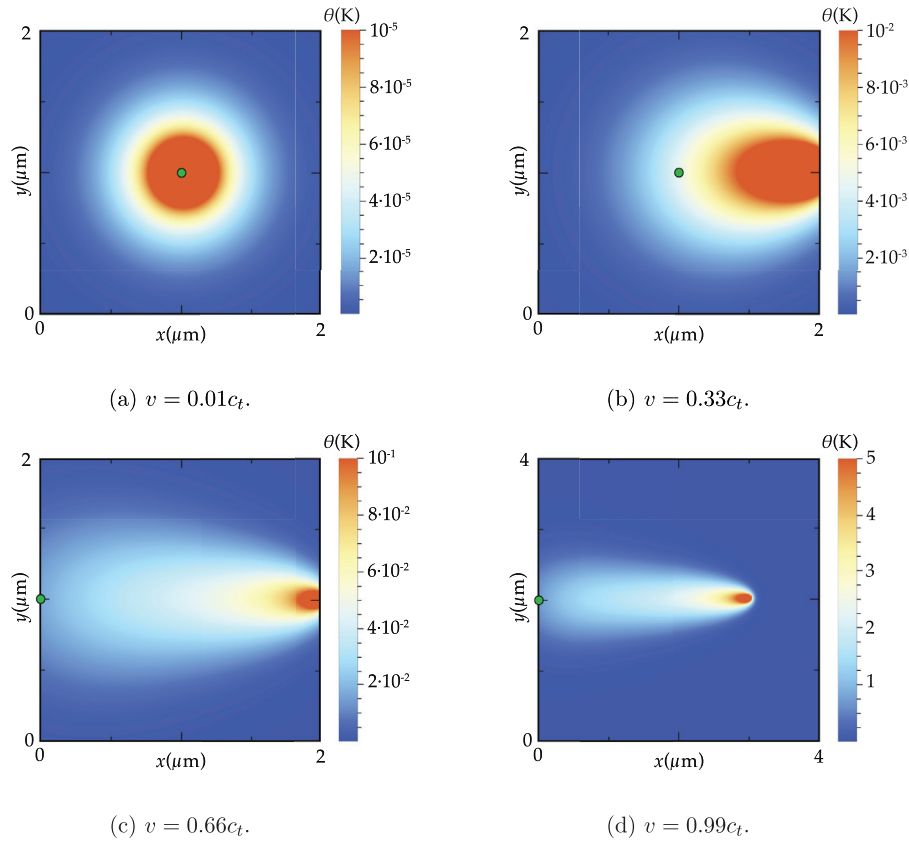


Fig. 1. Temperature fields for a uniformly moving dislocation, relative to a base temperature $T_0 = 298$ K. The parameters of pure aluminium have been used, with $K = 205$ W/m K, $c_t = 2980$ m/s, $\kappa_v = 9.7 \times 10^{-5}$ m²/s, $d_0 = 2 \times 10^{-5}$ Pas. The initial position of the dislocation is marked with a green circle, and it moves in the x direction at the specified uniform speed. The plots display the resulting temperature field at instant $t = 1$ ns. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

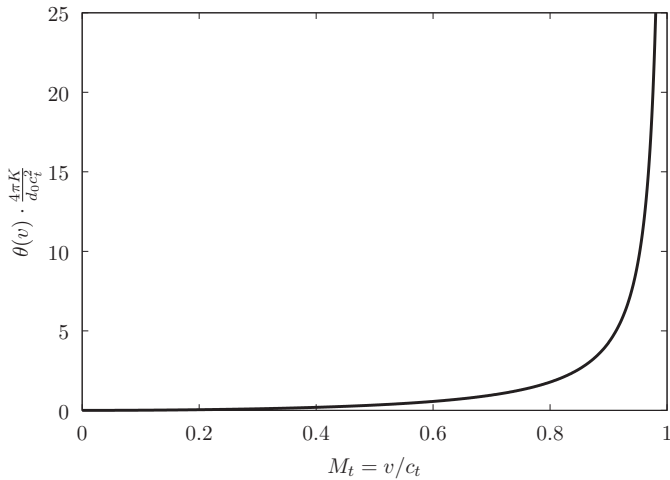


Fig. 2. Evolution of the temperature field of a moving dislocation in the immediacy of the core of the dislocation.

where σ_{ij} is the Cauchy stress tensor, and Λ and μ are respectively Lamé's first and second constants.⁵

Conservation of linear momentum is enforced by invoking Newton's second law, which in this case takes the form (Mura, 1982):

$$\sigma_{ij,j} + f_i = \rho \ddot{u}_i \quad (27)$$

⁵ Thus, μ is the shear modulus.

where f_i is any one body force, here assumed to not be present for simplicity, ρ is the material's density, and u_i denotes the displacement field components, so that $(x_1, x_2, x_3) \equiv (x, y, z)$. Here repeated index denotes summation, and $f_{,j} = \frac{\partial f}{\partial x_j}$; time derivatives are denoted using Newton's dot notation, i.e., $\dot{f} = \frac{\partial f}{\partial t}$.

Substituting the modified Hooke's law (Eq. (26)) over the equation of conservation of linear momentum (Eq. (27)) leads to the thermoelastic Navier-Lamé equation

$$(\Lambda + \mu)u_{j,ji} + \mu u_{i,jj} - \alpha_L(3\Lambda + 2\mu)\theta_{,i} = \rho \ddot{u}_i \quad (28)$$

In the thermoelastic system, heat transport is allowed to occur. It is assumed that heat flow is governed by Fourier's law (i.e., Eq. (1)), which in the thermoelastic problem must be modified to account for heat sources driven by volumetric changes (see Chadwick, 1960; Sneddon, 1972):

$$K\theta_{,kk} = \rho c_v \dot{\theta} + (3\Lambda + 2\mu)\alpha_L T_0 \dot{\epsilon}_{kk} \quad (29)$$

Eqs. (28) and (29) conform the coupled thermo-elastodynamic system of equations that govern the system's heat and momentum transport.

3.1.1. Uncoupling of the dynamic thermoelastic problem

The general uncoupling of the system of equations defined by Eqs. (28) and (29) is possible by invoking the Kelvin potentials, which requires expressing the displacement as the sum of a dilatational and an equivoluminal potential:

$$u_i = \phi_{,i} + \epsilon_{ijk}\psi_{k,j} \quad (30)$$

where ϕ is the dilatational potential (a scalar) and ψ the equivoluminal potential (a vector). In index notation, and where ϵ_{ijk} is the

Levi-Civita symbol. For the 2D case under consideration here, the edge dislocation is assumed to be moving along the x axis in the $x-y$ plane, so that the equivoluminal potential can be reduced to a single component, i.e. $\psi \equiv (0, \psi_y, 0)^T$. For simplicity, hereafter $\psi_y \equiv \psi$.

In that case, the displacement field components may be expressed as:

$$u_x = \frac{\partial \phi}{\partial x} - \frac{\partial \psi}{\partial y}, \quad u_y = \frac{\partial \phi}{\partial y} + \frac{\partial \psi}{\partial x}, \quad u_z = 0 \quad (31)$$

Substituting Eq. (31) into the thermo-elastic governing equations (Eqs. (28) and (29)), it is found that

$$(\Lambda + 2\mu)\nabla^2 \phi - \alpha_L(3\Lambda + 2\mu)\theta = \rho \ddot{\phi} \quad (32)$$

$$\rho \frac{\partial^2 \psi}{\partial t^2} = \mu \nabla^2 \psi \quad (33)$$

$$\rho c_v \dot{\theta} + \alpha T_0(3\Lambda + 2\mu) \frac{\partial}{\partial t} \nabla^2 \phi = K \nabla^2 \theta \quad (34)$$

The temperature field can be further uncoupled from the dilatational potential by extracting it from Eq. (32), so that:

$$\theta = \frac{1}{\alpha_L(3\Lambda + 2\mu)} ((\Lambda + 2\mu)\nabla^2 \phi - \rho \ddot{\phi}) \quad (35)$$

Substituting Eq. (38) into Eq. (34), the following fully uncoupled thermo-elastodynamic problem is reached:

$$\left[\nabla^2 - \aleph \frac{\partial}{\partial t} \right] [\nabla^2 \phi - a^2 \ddot{\phi}] = Q \nabla^2 (\dot{\phi}) \quad (36)$$

$$\nabla^2 \psi = b^2 \ddot{\psi} \quad (37)$$

$$\theta = (\Lambda + 2\mu) M_T (\nabla^2 \phi - a^2 \ddot{\phi}), \quad (38)$$

where

$$a^2 = \frac{\rho}{\Lambda + 2\mu}, \quad b^2 = \frac{\rho}{\mu}, \quad M_T = \frac{1}{\alpha_L(3\Lambda + 2\mu)}, \quad \aleph = \frac{\rho c_v}{K}, \quad Q = \frac{T_0}{K M_T^2 (\Lambda + 2\mu)} \quad (39)$$

Here, a and b are the athermal longitudinal and transverse slownesses of sound, respectively; \aleph the inverse of the material's thermal diffusivity at constant deformation; Q is a heat source rate term, and M_T a coupling term. Notice that

$$\epsilon = \frac{Q}{\aleph} \quad (40)$$

is the (dimensionless) thermoelastic coupling constant (see Chadwick, 1960), which serves as a measure of the strength of the coupling between the elastodynamic and thermal fields. When $\epsilon = 0$, the dilatational field in Eq. (36) is unaffected by the temperature field, and in the case of the injected, moving dislocation the problem reverts to the classical elastodynamic problem solved in Markenscoff and Clifton, 1981 and Gurrutxaga-Lerma et al., 2013. For most metals, $\epsilon \approx O(-2) - O(-3)$, meaning that the coupling is generally weak (Chadwick, 1960).

It is important to notice that the equivoluminal field equation (Eq. (37)) is fully uncoupled and does not directly impart on the temperature field (Eq. (38)). Thus, in the thermoelastic problem under consideration here, temperature changes will drive and be driven by dilatational changes in volume alone; further heat release via phonon dispersion will not be accounted for in this model.

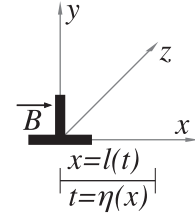


Fig. 3. Thermoelastic system. The dislocation of Burgers vector B is injected at the origin, and glides along the x axis following a certain $x = l(t)$ history. The system's material properties are its two elastic Lamé constants Λ and μ , its density ρ , its linear expansion coefficient α and its thermal conductivity K .

3.2. Boundary conditions

The boundary conditions of interest here are those describing the injection and motion of a straight edge dislocation along the x -axis. As is depicted in Fig. 3, x is assumed to be the glide direction. As discussed in Markenscoff and Clifton (1981) and Gurrutxaga-Lerma et al. (2013), this process can be modelled as:

$$u_x(x, y = 0, t) = \frac{B}{2} H(l(t) - x) H(t) \quad (41)$$

where $l(t)$ is the past history function that stores the position of the dislocation relative to the origin of coordinates over each instant t , and B the magnitude of the Burgers vector. For mathematical convenience (see Gurrutxaga-Lerma et al., 2013), this problem may be divided into the superposition of the following two:

1. An injected, quiescent dislocation, described by

$$u_x(x, y = 0, t) = \frac{B}{2} H(-x) H(t) \quad (42)$$

2. An injected dipole, one of which dislocations remains quiescent while the other glides according to $l(t)$:

$$u_x(x, y = 0, t) = \frac{B}{2} (H(l(t) - x) - H(-x)) H(t) \quad (43)$$

Two additional boundary conditions have to be enforced. First of all, in order to ensure that the normal stress is zero on the slip plane as a result of the injection and motion of the dislocation, it is specified that

$$\sigma_{yy}(x, y = 0, t) = 0 \quad (44)$$

Equally, in order to ensure the symmetry of the thermal field about the glide plane,

$$\frac{\partial \theta(x, y = 0, t)}{\partial y} = 0 \quad (45)$$

All boundary conditions apply for $t > 0$; for $t < 0$ the system is assumed to be undisturbed, i.e., $u_i = 0$ and $\theta = 0 \forall (x, y) \in \mathbb{R}^2$.

3.3. Solution in the Laplace domain for the injected, quiescent dislocation

The quiescent dislocation problem, i.e., the problem when $l(t) = 0$, is studied first. This describes the creation (injection) of a new dislocation that does not move afterwards. The relevant displacement boundary condition is given by Eq. (42), i.e.,

$$u_x(x, y = 0, t) = \frac{B}{2} H(-x) H(t)$$

In order to solve this problem, one may define the following sequence of unilateral and bilateral Laplace transforms:

$$\hat{f}(x, y, s) = \int_0^\infty f(x, y, t) e^{-st} dt, \quad (46)$$

$$F(\lambda, y, s) = \int_{-\infty}^{\infty} \hat{f}(x, y, s) e^{-\lambda s x} dx, \quad (47)$$

and apply them over both the governing equations (Eqs. (36) and (37)), which respectively leads to the following equations

$$\frac{\partial^4 \Phi}{\partial y^4} + (2\lambda^2 s^2 - a^2 s^2 - \aleph s - Qs) \frac{\partial^2 \Phi}{\partial y^2} + (-\alpha^2 \lambda^2 s^4 + \aleph s^3 \alpha^2 - Qs^3 \lambda^2) \Phi = 0 \quad (48)$$

$$\frac{\partial^2 \Psi}{\partial y^2} = \beta^2 s^2 \Psi \quad (49)$$

where $\alpha^2 = a^2 - \lambda^2$ and $\beta^2 = b^2 - \lambda^2$.

The solution to both equations is immediate:

$$\Phi = C_{\phi_+} e^{-p_+ y} + C_{\phi_-} e^{-p_- y} + C_{\phi_1} e^{p_+ y} + C_{\phi_2} e^{p_- y} \quad (50)$$

and

$$\Psi = C_{\psi} e^{-s\beta y} + C'_{\psi} e^{s\beta y} \quad (51)$$

Here p_{\pm} are the positive values of the solutions to equation

$$p^4 + (2\lambda^2 s^2 - a^2 s^2 - \aleph s - Qs) p^2 + (\aleph s^3 \alpha^2 - \lambda^2 s^4 \alpha^2 - Q\lambda^2 s^3) = 0, \quad (52)$$

which can be expressed as

$$p_{\pm} = \frac{+1}{\sqrt{2}} \sqrt{-A \pm \sqrt{A^2 - 4B}} \quad (53)$$

with

$$A = 2\lambda^2 s^2 - a^2 s^2 - \aleph s - Qs, \quad B = \aleph s^3 \alpha^2 - \lambda^2 s^4 \alpha^2 - Q\lambda^2 s^3 \quad (54)$$

Crucially, it must be noted that $p_{\pm} = p_{\pm}(\lambda, s)$.

In order to ensure the stability of the solutions, the latter must vanish as $y \rightarrow \infty$. Invoking the Laplace transform's final value theorem, this renders $C_{\phi_1} = C_{\phi_2} = C'_{\psi} = 0$. Thus, the solutions are reduced to

$$\begin{aligned} \Phi(\lambda, y, s) &= C_{\phi_+}(\lambda, s) e^{-p_+ y} + C_{\phi_-}(\lambda, s) e^{-p_- y}, \\ \Psi(\lambda, y, s) &= C_{\psi}(\lambda, s) e^{-s\beta y} \end{aligned} \quad (55)$$

The values of the integration constants C_{ϕ_+} , C_{ϕ_-} , and C_{ψ} can be obtained from the boundary conditions.

The σ_{yy} stress component in this case is of the form

$$\begin{aligned} \sigma_{yy}(x, y, t) &= \Lambda(u_{y,y} + u_{x,x}) + 2\mu u_{y,y} - (3\Lambda + 2\mu)\alpha_L \theta \\ &= (\Lambda + 2\mu)(\phi_{,yy} + \psi_{,xy}) + \lambda(\phi_{,xx} - \psi_{,xy}) \\ &\quad - (3\Lambda + 2\mu)\alpha_L \theta \end{aligned} \quad (56)$$

After some manipulations, this can be reduced to

$$\sigma_{yy}(x, y, t) = 2\mu(\psi_{,xy} - \phi_{,xx}) + \rho \ddot{\phi} \quad (57)$$

Applying the sequential Laplace transforms, one obtains the following boundary condition

$$\Sigma_{yy}(\lambda, 0, t) = 2\lambda s \left(\frac{\partial \Psi}{\partial y} - \lambda s \Phi \right) + b^2 s^2 \Phi = 0 \quad (58)$$

Substituting the solutions in,

$$(b^2 - 2\lambda^2) s^2 C_{\phi_+} + (b^2 - 2\lambda^2) s^2 C_{\phi_-} - 2\lambda \beta s^2 C_{\psi} = 0 \quad (59)$$

Equally, the other two field variables giving a boundary condition can be expressed in terms of the dilatational and equivoluminal potentials. The displacement boundary condition is

$$u_x(x, y = 0, t) = \phi_{,x} - \psi_{,y} = \frac{B}{2} H(-x) H(t) \quad (60)$$

which leads to

$$\lambda s C_{\phi_+} + \lambda s C_{\phi_-} + \beta s C_{\psi} = \frac{B}{2\lambda s^2} \quad (61)$$

The temperature boundary condition is

$$\frac{\partial \theta(x, y = 0, t)}{\partial y} = (\Lambda + 2\mu) M_T \frac{\partial}{\partial y} (\nabla^2 \phi - a^2 \ddot{\phi}) = 0 \quad (62)$$

which leads to

$$p_+(p_+^2 - \alpha^2 s^2) C_{\phi_+} + p_-(p_-^2 - \alpha^2 s^2) C_{\phi_-} = 0 \quad (63)$$

Eqs. (59), (61) and (63) form a linear system of equations

$$\begin{bmatrix} (b^2 - 2\lambda^2) s^2 & (b^2 - 2\lambda^2) s^2 & -2\lambda \beta s^2 \\ \lambda s & \lambda s & \beta s \\ p_+(p_+^2 - \alpha^2 s^2) & p_-(p_-^2 - \alpha^2 s^2) & 0 \end{bmatrix} \cdot \begin{bmatrix} C_{\phi_+} \\ C_{\phi_-} \\ C_{\psi} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{B}{2\lambda s^2} \\ 0 \end{bmatrix}, \quad (64)$$

the solution of which is the following:

$$C_{\phi_+}(\lambda, s) = \frac{B p_-(p_-^2 - \alpha^2 s^2)}{b^2 s^3 (p_- - p_+) (p_-^2 + p_- p_+ + p_+^2 - \alpha^2 s^2)} \quad (65)$$

$$C_{\phi_-}(\lambda, s) = -\frac{B p_+(p_+^2 - \alpha^2 s^2)}{b^2 s^3 (p_- - p_+) (p_-^2 + p_- p_+ + p_+^2 - \alpha^2 s^2)} \quad (66)$$

$$C_{\psi}(\lambda, s) = \frac{B(2\lambda^2 - b^2)}{2b^2 \beta \lambda s^3} \quad (67)$$

The inversion of the equivoluminal potential is immediate employing the Cagniard-de Hoop technique, and leads to the solutions for the shear wave component of the injected dislocation provided by Gurrutxaga-Lerma et al. (2013). As expected, it does not affect the dilatational and temperature fields.

3.3.1. The temperature field

Consider the thermal field in the Laplace domain

$$\Theta(\lambda, y, s) = \frac{1}{s^3} F(\lambda, s) (p_+ e^{-p_+ y} - p_- e^{-p_- y}) \quad (68)$$

where

$$F(\lambda, s) = \frac{B M_T (\Lambda + 2\mu)}{b^2} \frac{(p_-^2 - \alpha^2 s^2) (p_+^2 - \alpha^2 s^2)}{(p_- - p_+) (p_-^2 + p_- p_+ + p_+^2 - \alpha^2 s^2)} \quad (69)$$

The spatial inversion will be:

$$\hat{\theta}(x, y, s) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \frac{1}{s^2} F(\lambda, s) (p_+ e^{-p_+ y} - p_- e^{-p_- y}) e^{s\lambda x} d\lambda \quad (70)$$

In the expression above, the integrand has exponential factors that may be expressed as

$$e^{-s(q_{\pm} y - \lambda x)}, \quad (71)$$

where for convenience, $p_{\pm} = sq_{\pm}$, i.e.,

$$q_{\pm} = \sqrt{-\lambda^2 + \frac{a^2 s + \aleph + Q \pm \sqrt{2\aleph(Q - a^2 s) + (a^2 s + Q)^2 + \aleph^2}}{2s}} \quad (72)$$

This is reminiscent of a Cagniard-de Hoop kernel (see De Hoop, 1960). However, q_{\pm} is dependent on both s and λ , so the inversion cannot be directly performed over a conventional Cagniard path.

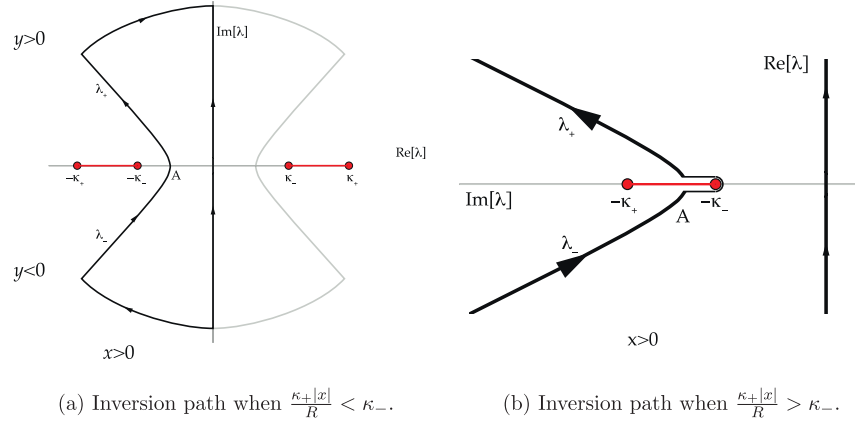


Fig. 4. Inversion paths.

Still, one can define a contour along which the exponential factor takes the form

$$e^{-s\tau} \quad (73)$$

where

$$\tau = q_{\pm}y - \lambda x \quad (74)$$

Thus, the integration variable can be expressed in terms of τ by making the following change of variable:

$$\lambda = \frac{-\tau x \pm iy \sqrt{\tau^2 - R^2 \frac{a^2 s + \aleph + Q \pm \sqrt{2\aleph(Q - a^2 s) + (a^2 s + Q)^2 + \aleph^2}}{2s}}}{R^2} \quad (75)$$

where $R^2 = x^2 + y^2$.

For convenience however, it is best to regroup variables as follows

$$\lambda = \frac{-\tau x \pm iy \sqrt{\tau^2 - \kappa_{\pm}^2 R^2}}{R^2} \quad (76)$$

where

$$\kappa_{\pm}^2 = \frac{a^2 s + \aleph + Q \pm \sqrt{2\aleph(Q - a^2 s) + (a^2 s + Q)^2 + \aleph^2}}{2s} \quad (77)$$

It is easy to check that for $s > 0$, $\kappa_+ > \kappa_-$. In the following, when invoking λ , κ_+ will be applied for the e^{-p+y} integral, and κ_- for the e^{-p-y} integral. This means that for each of those two branch, p_{\pm} takes different values, since $p_{\pm} = s\sqrt{\kappa_{\pm}^2 - \lambda}$ explicitly depends on λ .

For clarity, here the case of e^{-p+y} will be discussed; analogous reasoning can be extended to the case of e^{-p-y} . Thus, here the following λ will be considered:

$$\lambda_{\pm} = \frac{-\tau x \pm iy \sqrt{\tau^2 - \kappa_{\pm}^2 R^2}}{R^2} \quad (78)$$

As in the standard Cagniard-de Hoop path (see Gurrutxaga-Lerma et al., 2013), Eq. (78) describes a parametrised hyperbola in the complex λ plane. The following convention will be used here. For $y > 0$, the λ_+ branch is in the upper half plane ($\text{Im}[\lambda] > 0$), and the λ_- branch in the lower half plane ($\text{Im}[\lambda] < 0$). In this same convention, the $x < 0$ branches are the branches in the right half plane (for which $\text{Re}[\lambda] > 0$); for $x > 0$, the branches are in the left half plane. This is shown in Fig. 4a.

The intersection of the hyperbola with the real axis will define its vertex, which is found when $\text{Im}[\lambda_{\pm}] = 0$. At that point, the variable τ takes the value $+\kappa_+R$, whilst the real part of λ_{\pm} is $-\tau x/R$. This defines a vertex 'A' at

$$\lambda_A = -\frac{x\kappa_+}{R} \quad (79)$$

As λ_+ moves from λ_A towards the asymptote of the corresponding λ_+ branch, the value of τ goes from $+\kappa_+R$ at the vertex to $\tau \rightarrow \infty$ at the asymptotic limit. This remains analogous for the $y < 0$ branches.

Thus, the hyperbolic path in the λ plane is mapped onto a path along the real axis of the τ plane, with $\tau \in [+\kappa_+R, \infty)$. In this sense, the present integration path mirrors a Cagniard-de Hoop inversion path.

Particularly care must be taken to avoid branch cuts and poles in the integrand, which is of the form

$$p_+ \frac{(p_-^2 - \alpha^2 s^2)(p_+^2 - \alpha^2 s^2)}{(p_- - p_+)(p_-^2 + p_- p_+ + p_+^2 - \alpha^2 s^2)}$$

The integrand has poles when its denominator cancels, which occurs for

$$\lambda_{1,2} = \pm \frac{\sqrt{2a^2(\kappa_-^2 + \kappa_+^2) - a^4 - \kappa_-^4 - \kappa_-^2 \kappa_+^2 - \kappa_+^4}}{\sqrt{2a^2 - \kappa_-^2 - \kappa_+^2}}$$

In principle, $|\lambda_{1,2}| > \lambda_A$ for $\kappa_+ > \kappa_-$, which means the poles leave no residue.

In addition, the integrand has branch cuts defined for $\text{Im}[\lambda] = 0$, $\text{Re}[\lambda] \in (-\kappa_-, \kappa_-) \cap (-\kappa_+, \kappa_+)$. The branch cut may therefore be crossed for values of x such that $|\lambda_A| = \frac{\kappa_+|x|}{R} > \kappa_-$. When this occurs, λ has only a real part, defined by

$$\lambda^* = \frac{-\tau x + y \sqrt{\kappa_+^2 R^2 - \tau^2}}{R^2} \quad (80)$$

Necessarily, this specifies that $\kappa_+^2 R^2 > \tau^2$, and since $\frac{\kappa_+|x|}{R} > \kappa_-$, the values τ may take here can be parametrised as

$$\tau \in (\kappa_-x + y\sqrt{\kappa_+^2 - \kappa_-^2}, +\kappa_+R) \quad (81)$$

This entails that when $\frac{\kappa_+|x|}{R} > \kappa_-$ (in general, for very small values of x and y in close proximity to the dislocation's injection site), the contour defined by the λ_{\pm} hyperbola branch must be extended to include the values defined in Eq. (80).

With this in place, the contour along the imaginary axis defined in Eq. (70) can be distorted in a way akin to the Cagniard-de Hoop technique. The complete contour is shown in Fig. 4a. For either $x > 0$ or $x < 0$, a closed contour of integration in the λ plane will be defined, formed by the corresponding side of the imaginary axis, the λ_- and λ_+ hyperbola branches that meet at λ_A (corresponding, respectively, to the lower and upper half planes); the asymptotes of the hyperbola branches are joined together with the imaginary axis via a circular contour at infinity. The latter's contribution to the value of the closed contour integral is zero by proper-

ties of the Laplace transform. Thus, as in Cagniard's method, invoking Cauchy's integral theorem the integral along the imaginary axis (the one in Eq. (70)) will be of the same value as the one along the hyperbola branches, which in turn describes an integration along the real axis of the τ plane in the interval $\tau \in [\kappa_+ R, \infty)$. If $\frac{\kappa_+ |x|}{R} > \kappa_-$, then the contour must be modified to avoid the branch cut in the way described in Fig. 4b, and outlined above in Eq. (80). The case of $x < 0$ is entirely analogous, and so is the case of e^{-p-y} , with the exception that in the latter κ_- must be used where κ_+ was used here.

Although agreeable to be written in Cagniard form, the contour defined above is not a classical Cagniard path because q_{\pm} and by extension, κ_{\pm} , depend on s . One can still write the inversion integral in time as a single integral

$$\hat{\theta}(x, y, s) = \frac{1}{\pi} \text{Im} \left[\int_{R\kappa_+}^{\infty} \left[\frac{\partial \lambda_+}{\partial \tau} \frac{1}{s^2} F(\lambda_+, s) p_+ e^{-s\tau_+} \right]_{\lambda_+, \kappa_+} d\tau - \int_{R\kappa_-}^{\infty} \left[\frac{\partial \lambda_-}{\partial \tau} \frac{1}{s^2} F(\lambda_-, s) p_- e^{-s\tau_-} \right]_{\lambda_-, \kappa_-} d\tau \right] \quad (82)$$

The case when $\frac{\kappa_+ |x|}{R} > \kappa_-$ only affects the first integral (for the second, $\kappa_- |x|/R < \kappa_+$ always). In that case, following Eq. (81) the first integral must be extended as follows:

$$\hat{\theta}^*(x, y, s) = \frac{1}{\pi} \text{Im} \int_{R\kappa_+}^{R\kappa_+} \left[\frac{\partial \lambda^*}{\partial \tau} \frac{1}{s^2} F(\lambda^*, s) p_+ e^{-s\tau_+} \right]_{\lambda^*, \kappa_+} d\tau \times H\left(\frac{\kappa_+ |x|}{R} - \kappa_-\right)$$

where λ^* is given by Eq. (80).

The inversion of this integral is challenging because s cannot be extracted from the integrand (nor from the integration limits), and therefore the latter cannot be written in a Cagniard form. In general, the inversion would be

$$\theta(x, y, t) = \frac{1}{2\pi i} \int_{\text{Br}} \left[\hat{\theta}^* + \frac{1}{\pi} \text{Im} \left[\int_{R\kappa_+}^{\infty} \left[\frac{\partial \lambda_+}{\partial \tau} \frac{1}{s^2} F(\lambda_+, s) p_+ e^{-s\tau_+} \right]_{\lambda_+, \kappa_+} d\tau - \int_{R\kappa_-}^{\infty} \left[\frac{\partial \lambda_-}{\partial \tau} \frac{1}{s^2} F(\lambda_-, s) p_- e^{-s\tau_-} \right]_{\lambda_-, \kappa_-} d\tau \right] e^{st} ds \right] \quad (83)$$

The general, closed form solution to Eq. (83) is probably unachievable in view of the fact that κ_{\pm} is a function of the transformed parameter s . However, one can still achieve asymptotic solutions to the temperature field by invoking the Abelian-Tauberian theorems of the Laplace transform (see Feller, 1968).

The small times behaviour of the temperature field can be deduced as follows. According to the Abelian theorem,

$$\lim_{t \rightarrow 0} \theta(t; x, y) = \lim_{s \rightarrow \infty} s \hat{\theta}(s; x, y) \quad (84)$$

It is easy to check that in that limit, the integrands in Eq. (83) tend to 0, which simply guarantees that the temperature field is initially undisturbed. The converse Tauberian theorem can also be applied to check the stability of the solution given by Eq. (83) at $t \rightarrow \infty$, which guarantees that $\lim_{t \rightarrow \infty} \theta(t; x, y) = 0$ as well. Since the thermal field is diffusive in nature, this means that after a transient, the temperature in the system will return to its initial values.

Asymptotic expansions employing the Abelian theorem enable us to estimate the magnitude of the early temperature transients. In the limit of $s \rightarrow \infty$, $\kappa_+ \rightarrow a$ and $\kappa_- \rightarrow 0$, so the integral becomes

$$\lim_{s \rightarrow \infty} s \hat{\theta}(x, y, s) = \lim_{s \rightarrow \infty} \frac{1}{\pi} \text{Im} \left[\int_{+Ra}^{\infty} \left[\frac{\partial \lambda_+}{\partial \tau} \frac{1}{s} F(\lambda_+, s) p_+ e^{-s\tau_+} \right]_{\lambda_+, \kappa_+} d\tau - \int_0^{\infty} \left[\frac{\partial \lambda_-}{\partial \tau} \frac{1}{s} F(\lambda_-, s) p_- e^{-s\tau_-} \right]_{\lambda_-, \kappa_-} d\tau \right] \quad (85)$$

The variables p_{\pm} are expanded in Taylor series of $1/s$ about $1/s = 0^+$ (i.e., about $s \rightarrow \infty$) (cf. Chadwick, 1960) which yields (to first order)

$$p_+ \approx \alpha s + \frac{Q}{2\alpha} + O(s^{-1}) \quad (86)$$

$$p_- \approx -i\lambda s - i\frac{\aleph}{2\lambda} + O(s^{-1}) \quad (87)$$

Substituting in the integrands in the Abelian limit, one can reach an asymptotic expression to first order in t of the form

$$\theta \approx \frac{BM_T(\Lambda + 2\mu)a^2}{\pi b^2} \frac{y}{R^2} \sqrt{t^2 - a^2 R^2} H(t - Ra) \quad (88)$$

The $\frac{y}{R^2}$ factor corresponds with the geometric factor that governs the hydrostatic pressure field around the core of a dislocation (see Hirth and Lothe, 1982). Thus, Eq. (88) shows that in the immediacy of the core, the temperature field around is homologous to the hydrostatic pressure field that, in fact, causes it.

The magnitude of the initial temperature field around the dislocation can therefore be estimated from Eq. (88). For aluminium, at a distance of about 100B from the core over very short timescales ($t \approx 1$ ps), the temperature increase may be estimated at around 1K, for a previously undeformed unbounded solid where a dislocation has just been injected. This transient heating effect is often observed in molecular dynamics simulations of dislocations: in the equilibration of an atomistic system with a dislocation, one often observes an initial transient heating that quickly dies out (cf. Gilbert et al., 2011).

The small magnitude of the thermomechanical heating is in agreement with previous estimates of this effect, such as those by Lothe (1962), and must be attributed to the weak coupling between the thermal and mechanical fields, which is conventionally measured via ϵ .

Lessen (1956) proposed that any thermoelastic problem may be studied perturbatively by expanding the Kelvin potentials in series of the coupling constant about $\epsilon = 0$. Albeit this approach hardly ever leads to a practical solution of the problem at hand, it enables the study the effect of the weakness of the coupling in the current situation. Accordingly, the solutions p_{\pm} are expanded in terms of the ϵ , which leads to

$$p_+ \approx \sqrt{s(\aleph - l^2 s)} + \frac{\aleph^2 s}{2(\aleph - a^2 s)\sqrt{s(\aleph - l^2 s)}} \epsilon - \frac{(\aleph^3 s^2 (3a^2 \aleph s - 4a^2 l^2 s^2 + \aleph^2))}{8((\aleph - a^2 s)^3 (s(\aleph - l^2 s))^{3/2})} \epsilon^2 + O(\epsilon^3)$$

$$p_- \approx \alpha s - \frac{a^2 \aleph s}{2\alpha(\aleph - a^2 s)} \epsilon + \frac{a^2 \aleph^2 s (3a^2 \aleph - 4\aleph l^2 + a^4 s)}{8\alpha^{3/2}(\aleph - a^2 s)^3} \epsilon^2 + O(\epsilon^3)$$

Taking this onto Eq. (55), it will be found that the dilatational potential in the Laplace domain may be written as

$$\Phi = \Phi_0 + \Phi_1 \epsilon + O(\epsilon^2)$$

where Φ_0 is Φ for the case when $\epsilon = 0$. In that case, the solutions in the Laplace domain (Eq. (55)) undergo heavy simplifications; in

particular

$$\Phi_{\epsilon \rightarrow 0} = \frac{B}{b^2 s^3} e^{-s\alpha y}$$

because $C_{\phi_+} = 0$ when $\epsilon = 0$. This Φ_0 happens to be the solution for the dilatational potential in the uncoupled problem (see Gurrutxaga-Lerma et al., 2013), which is discussed in detail in Section 4. The form of Ψ_1 is lengthy and protracted, and does not allow for a direct inversion. Still, it can be approximated as a series expansion in time, the first order term of which is $O(t^{-1/2})$; this entails that the ratio $\psi_1/\psi_0 \approx t^{-3/2}$, which indicates that the first order perturbation will be very small compared with the uncoupled solution ψ_0 , and therefore that the influence of the thermoelastic coupling will be small. As remarked by Boley and Weiner (1960), the relative weakness of the coupling is consistent with the nature of the loading rate, which in the present case, and at a sufficient distance away from the dislocation core (where the elastodynamic solution itself becomes invalid (Hirth and Lothe, 1982)) and away from the injection fronts (where, again, a weak divergence takes place (Gurrutxaga-Lerma et al., 2014)), is going to be very similar to that of the temperature, so that the coupling is going to be weak. This is driven by the fact that the thermal perturbations are brought about by the dilatational fields.

3.4. Solution in Laplace domain for the injected, moving dislocation

The moving dislocation is modelled via the appropriate boundary condition,

$$u_x(x, y = 0, t) = \frac{B}{2} H(l(t) - x) H(t) \quad (89)$$

where as mentioned above $l(t)$ is the past history function. Following Markenscoff (1980), it is more convenient to rewrite this as

$$u_x(x, 0, t) = \frac{B}{2} (H(\eta(x) - t) - H(-x)) H(t) + \frac{B}{2} H(-x) H(t) \quad (90)$$

where $l^{-1}(t) \equiv \eta(x)$ is the inverse past history function, i.e., the function that returns the instant in time when the dislocation core reaches position x . The second summing term on the right hand side correspond with the injection of a quiescent dislocation which was solved before; here only the problem associated with the first summing term in Eq. (90) will be solved, i.e.,

$$u_x(x, 0, t) = \frac{B}{2} (H(\eta(x) - t) - H(-x)) H(t) \quad (91)$$

Upon transforming u_x to the Laplace domain, one can construct the following system of equations and associated solutions to the governing equations:

$$\begin{bmatrix} (b^2 - 2\lambda^2)s^2 & (b^2 - 2\lambda^2)s^2 & -2\lambda\beta s^2 \\ \lambda s & \lambda s & \beta s \\ p_+(p_+^2 - \alpha^2 s^2) & p_-(p_-^2 - \alpha^2 s^2) & 0 \end{bmatrix} \cdot \begin{bmatrix} C_{\phi_+} \\ C_{\phi_-} \\ C_{\psi} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{B}{2s} \int_0^\infty e^{-s(\eta(\xi) + \lambda\xi)} d\xi \\ 0 \end{bmatrix}, \quad (92)$$

the solution of which is the following:

$$C_{\phi_+}(\lambda, s) = \frac{B\lambda p_-(p_-^2 - \alpha^2 s^2)}{b^2 s^2 (p_- - p_+) (p_-^2 + p_- p_+ + p_+^2 - \alpha^2 s^2)} \times \int_0^\infty e^{-s(\eta(\xi) + \lambda\xi)} d\xi \quad (93)$$

$$C_{\phi_-}(\lambda, s) = -\frac{B\lambda p_+(p_+^2 - \alpha^2 s^2)}{b^2 s^2 (p_- - p_+) (p_-^2 + p_- p_+ + p_+^2 - \alpha^2 s^2)} \times \int_0^\infty e^{-s(\eta(\xi) + \lambda\xi)} d\xi \quad (94)$$

$$C_{\psi}(\lambda, s) = \frac{B(2\lambda^2 - b^2)}{2b^2 \beta s^2} \int_0^\infty e^{-s(\eta(\xi) + \lambda\xi)} d\xi \quad (95)$$

In the particular case when $l(t) = v \cdot t$, i.e., when the dislocation glides with uniform speed v , the system is amenable to a more explicit solution. In that case, $\eta(x) = x/v = dx$, for $d = 1/v$ the dislocation's glide slowness, whereby the coefficients of the solution are

$$C_{\phi_+}(\lambda, s) = \frac{B\lambda p_-(p_-^2 - \alpha^2 s^2)}{b^2 s^3 (\lambda + d) (p_- - p_+) (p_-^2 + p_- p_+ + p_+^2 - \alpha^2 s^2)} \quad (96)$$

$$C_{\phi_-}(\lambda, s) = -\frac{B\lambda p_+(p_+^2 - \alpha^2 s^2)}{b^2 s^3 (\lambda + d) (p_- - p_+) (p_-^2 + p_- p_+ + p_+^2 - \alpha^2 s^2)} \quad (97)$$

$$C_{\psi}(\lambda, s) = \frac{B(2\lambda^2 - b^2)}{2b^2 \beta (\lambda + d) s^3} \quad (98)$$

The inversion follows same procedure outlined for the quiescent case, mimicking the Cagniard-de Hoop technique along the path defined by $\tau = q_{\pm} - \lambda x$. The same considerations related to the branch cuts in Fig. 4 apply; so long as $d > a$, the additional pole at $\lambda = d$ is never encountered along the integration path, so it will leave no residue. After careful manipulations, one reaches the following expression for the temperature field

$$\hat{\theta} = \hat{\theta}^* + \frac{1}{\pi} \text{Im} \left[\int_{\tau_{K_+}}^\infty \left[\frac{\partial \lambda_+}{\partial \tau} \frac{\lambda_+}{(\lambda_+ + d)} \frac{1}{s^2} F(\lambda_+, s) p_+ e^{-s\tau} \right]_{\lambda_+, K_+} d\tau - \int_{\tau_{K_-}}^\infty \left[\frac{\partial \lambda_+}{\partial \tau} \frac{\lambda_+}{(\lambda_+ + d)} \frac{1}{s^2} F(\lambda_+, s) p_- e^{-s\tau} \right]_{\lambda_+, K_-} d\tau \right] \quad (99)$$

where

$$F_{\pm}(s) = \frac{BM_T(\Lambda + 2\mu)}{b^2} \frac{(p_-^2 - \alpha^2 s^2)(p_+^2 - \alpha^2 s^2)}{(p_- - p_+) (p_-^2 + p_- p_+ + p_+^2 - \alpha^2 s^2)}$$

and

$$\hat{\theta}^*(x, y, s) = \frac{1}{\pi} \text{Im} \int_{K_- x + y \sqrt{K_+^2 - K_-^2}}^{RK_+} \times \left[\frac{\partial \lambda^*}{\partial \tau} \frac{\lambda_+}{(\lambda_+ + d)} \frac{1}{s^2} F(\lambda^*, s) p_+ e^{-s\tau} \right]_{\lambda^*, K_+} d\tau \times H\left(\frac{K_+ |x|}{R} - K_-\right) \quad (100)$$

As in the case of the injected dislocation, the greatest problem here is that $\tau = \tau(s)$. The inverted temperature field will be

$$\theta = \frac{1}{2\pi i} \int_{Br} \left[\hat{\theta}^* + \text{Im} \int_{\tau_{K_+}}^\infty \left[\frac{\partial \lambda_+}{\partial \tau} \frac{\lambda_+}{(\lambda_+ + d)} \frac{1}{s^2} F(\lambda_+, s) p_+ e^{-s\tau} \right]_{\lambda_+, K_+} d\tau - \int_{\tau_{K_-}}^\infty \left[\frac{\partial \lambda_+}{\partial \tau} \frac{\lambda_+}{(\lambda_+ + d)} \frac{1}{s^2} F(\lambda_+, s) p_- e^{-s\tau} \right]_{\lambda_+, K_-} d\tau \right] e^{st} dt \quad (101)$$

One may again invoke the Abelian theorem and perform an asymptotic expansion about $s \rightarrow \infty$ to find the small times behaviour of the solution. Using the same procedure as in the case of the injected, quiescent dislocation, one finds that

$$\theta(v) \approx -\frac{BM_T(\Lambda + 2\mu)Q}{\pi b^2} \frac{y}{R^2} \times \left(t - \text{sign}(y) \frac{\sqrt{d^2 - a^2}}{a} \arctan \left(\frac{t - dx}{y\sqrt{d^2 - a^2}} \right) \right) \quad (102)$$

Using the same approach the behaviour about the core ($R \rightarrow 0$) may also be inferred. If R is small, one may estimate $\hat{\theta}$ to be

$$\hat{\theta}(x, y, s) \approx \frac{BM_T(\Lambda + 2\mu)}{\pi b^2 s^2} \int_0^\infty \frac{-a^2 s^2 y (\tau - 2 dx)}{R^2 \tau (d^2 R^2 - 2 d\tau x + \tau^2)} e^{-s\tau} d\tau, \quad (103)$$

which is in Cagniard form, so that the time inversion can be performed by inspection:

$$\theta(x, y, t) \approx \frac{Ba^2 M_T(\Lambda + 2\mu)}{\pi b^2} \frac{y}{R^2} \frac{-t(t - 2 dx)}{(d^2 R^2 - 2 dtx + t^2)} \quad (104)$$

In this case, the magnitude of the temperature field increases with the dislocation's glide speed in an almost quadratic fashion. To a good approximation, for slow moving dislocations

$$\theta(x, y, t) \approx \frac{Ba^2 M_T(\Lambda + 2\mu)}{\pi b^2} \frac{y t v}{R^2} \left(\frac{t v (R^2 - 4x^2)}{R^4} - \frac{2x}{R^2} \right) \quad (105)$$

For slow moving dislocations, the thermomechanical temperature increase due to a moving dislocation will therefore approximately scale quadratically relative to the dislocation's speed.

One may again estimate the magnitude of the thermomechanical effect about the dislocation core, in this case motivated by a moving dislocation. The prefactor is in this case the same as in the injected case, so for Al it will be of the order of 10^{-6} Km; for a dislocation moving at low speeds ($v = 0.01c_t$), this entails a temperature rise at a distance of $100B$ about the core of about $1K$ for times of $t = 1$ ps; for a dislocation moving at $v = 0.99c_t$, the temperature raise is about $3.8K$. This temperature increase might seem unexpectedly small; however, it must be born in mind that whilst the limiting speed of the dislocation is the transverse speed of sound c_t , the representative speed of the dilatational field is the longitudinal speed of sound c_l , which is about twice as large: even a dislocation moving at the transverse speed of sound will still be moving at half the longitudinal speed of sound, which entails that the dilatational fields will hardly experience a Doppler-like contraction and, therefore, that the ensuing thermal field remains largely undisturbed by the dilatational field of the moving dislocation.

4. Approximating the thermomechanical field of a dislocation as an the uncoupled thermoelastic problem

As was found by Hetnarski (1964b; 1964a) and Nowacki (1975) for line sources, in the current study the strength of the coupling between the elastodynamic and the thermal fields is weak enough that the thermal field arising from the dilatational radiation of a moving source may be approximated by simply considering uncoupling the elastodynamic and the thermal fields in such a way that the latter remains excited by the dilatational field.

This means that the elastodynamic field will be fully uncoupled from the thermal field, so that the injection and motion of the edge dislocation may be described as done by Markenscoff and Clifton (1981) and Gurrutxaga-Lerma et al. (2013) for the case, respectively, of a non-uniformly moving edge dislocation and an injected edge dislocation.

In turn, the thermal field will be excited by the dilatational field (i.e., $\phi(x, y, t)$) the elastodynamic dislocation described in Markenscoff and Clifton (1981) and Gurrutxaga-Lerma et al. (2013) entail. This dilatational excitation ϕ triggers heating in the thermal field, which is simply governed by Eq. (38)

$$\theta = \frac{1}{\alpha(3\Lambda + 2\mu)} ((\Lambda + 2\mu)\nabla^2 \phi - \rho \ddot{\phi})$$

Notice that unlike in the fully coupled problem, here θ will not appear in the modified Hooke's law, and will therefore not contribute to the Navier–Lamé equation.

Specifically, the dilatational excitations of concern here may be found, in the Laplace domain, in Gurrutxaga-Lerma et al. (2013). For the injected dislocation, they are of the form

$$\Phi(\lambda, y, s) = \frac{B}{b^2 s^3} e^{-s\alpha y}, \quad (106)$$

For the non-uniformly moving dislocation, they are given by Gurrutxaga-Lerma et al. (2013),

$$\Phi(\lambda, y, s) = \frac{B\lambda}{b^2 s^2} \left[\int_0^\infty e^{-s(\eta(\xi) + \lambda\xi)} d\xi \right] e^{-s\alpha y}, \quad (107)$$

For the special case of a uniformly moving dislocation with speed $v = 1/d$, the dilatational potential in the Laplace domain takes the form (Gurrutxaga-Lerma et al., 2014)

$$\Phi(\lambda, y, s) = \frac{B}{b^2 s^3} \frac{\lambda}{\lambda + d} e^{-s\alpha y} \quad (108)$$

Throughout here, the same spatial variables and kinematic notation as in previous sections has been employed. Note that $\alpha^2 = a^2 - \lambda^2$.

This dilatational excitation, ϕ , triggers heating in the thermal field, which is simply governed by Eq. (38)

$$\theta = M_T ((\Lambda + 2\mu)\nabla^2 \phi - \rho \ddot{\phi})$$

whereupon in the Laplace domain,

$$\Theta = M_T (\Lambda + 2\mu) \left[\alpha^2 s^2 \Phi + \frac{\partial^2 \Phi}{\partial y^2} \right]$$

Substituting the expressions above, Eqs. (106), (107), and (108), one obtains respectively,

$$\Theta(\lambda, y, s) = M_T (\Lambda + 2\mu) \frac{2B}{b^2 s} \alpha^2 e^{-s\alpha y}, \quad (109)$$

$$\Theta(\lambda, y, s) = M_T (\Lambda + 2\mu) \frac{2B}{b^2 s} \alpha^2 \lambda \left[\int_0^\infty e^{-s(\eta(\xi) + \lambda\xi)} d\xi \right] e^{-s\alpha y} \quad (110)$$

$$\Theta(\lambda, y, s) = M_T (\Lambda + 2\mu) \frac{2B}{b^2 s} \alpha^2 \frac{\lambda}{\lambda + d} e^{-s\alpha y} \quad (111)$$

These expressions can be inverted immediately using Cagniard-de Hoop; no poles or extraneous branch cuts are observed, so the inversion follows the same integration contour as in Gurrutxaga-Lerma et al. (2013).

It is found that, for the case of the injected and uniformly moving dislocations, the Cagniard form is, respectively,

$$\begin{aligned} \hat{\theta}_{\text{injected}}(x, y, s) &= \frac{2BM_T(\Lambda + 2\mu)}{\pi b^2} \frac{1}{s} \\ &\times \int_0^\infty \frac{\tau y (3a^2 R^2 x^2 + \tau^2 (y^2 - 3x^2))}{R^6 \sqrt{\tau^2 - a^2 R^2}} \\ &\times H(t - Ra) e^{-s\tau} d\tau \end{aligned} \quad (112)$$

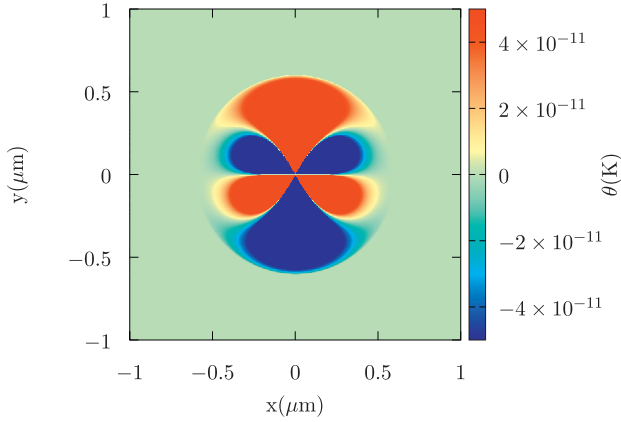


Fig. 5. Uncoupled temperature field for an injected edge dislocation. The dislocation was injected at the origin, and the instant in time represented is 0.1 ns; the material constants of FCC Al have been used.

and

$$\begin{aligned} \hat{\theta}_{\text{uniform}}(x, y, s) = & \frac{2BM_T(\Lambda + 2\mu)}{\pi b^2} \frac{1}{s} \\ & \times \int_0^\infty \frac{y d}{R^4 \sqrt{\tau^2 - a^2 R^2} (d^2 R^2 - 2d\tau x + \tau^2 - a^2 y^2)} \\ & \times (a^4 x^3 R^2 - 3a^2 d\tau x^2 R^2 + a^2 \tau^2 x(x^2 + 3y^2) \\ & + d\tau^3 (3x^2 - y^2) - 2\tau^4 x) H(\tau - Ra) e^{-s\tau} d\tau \quad (113) \end{aligned}$$

The final inversion in these two cases is immediate by invoking Laplace transform properties, which for the injected case render

$$\begin{aligned} \theta(x, y, t)_{\text{injected}} = & \frac{2BM_T(\Lambda + 2\mu)}{\pi b^2} \\ & \times \frac{y \sqrt{t^2 - a^2 R^2} (a^2 R^2 (3x^2 + 2y^2) + t^2 (y^2 - 3x^2))}{3R^6} \\ & \times H(t - aR) \quad (114) \end{aligned}$$

For the uniformly moving case, the resulting expression is too long to be contained in here, and is provided in the appendix.

The generally non-uniformly moving dislocation's case leads to

$$\theta(x, y, t)_{\text{non-uniform}} = \frac{2BM_T(\Lambda + 2\mu)}{\pi b^2} F_T(t)$$

where

$$F_T(t) = \int_0^\infty H(\tilde{t} - \tilde{R}a) G(\tilde{t}, \xi) d\xi$$

where $\tilde{t} = t - \eta(\xi)$, $\tilde{R}^2 = \tilde{x}^2 + y^2$, $\tilde{x} = x - \xi$ and

$$G(\tilde{t}, \xi) = \frac{y \sqrt{\tilde{t}^2 - a^2 \tilde{R}^2} (a^2 \tilde{R}^2 (3\tilde{x}^2 + 2y^2) + \tilde{t}^2 (y^2 - 3\tilde{x}^2))}{3\tilde{R}^3}$$

The resulting temperature fields can readily be evaluated. For distances far away from the core which are thermally excited at timescales of the order of 1 ns, the thermomechanical heating resulting from the dilatational fields of the dislocations is yet again observed to be of very small magnitude, irrespective of the speed of the dislocation. Fig. 5 shows the temperature field at a distance of $\approx 1 \mu\text{m}$ away from the core of an edge dislocation injected in FCC Al; as can be observed, at time 0.1 ns after the injection, the underlying rise in temperature as a result of the injection itself is entirely negligible ($O(-11)\text{K}$). The predicted heating only seems

to exceed $O(1)\text{K}$ for extremely short timescales (i.e., $< 1 \text{ ps}$), and only for positions of the order of 1 \AA (i.e., over one atomic distance away from the core, where the whole continuum treatment of the dislocation is invalid anyway). The magnitude of θ_{uniform} is directly proportional to the dislocation speed, and may be expanded to first order as

$$\begin{aligned} \theta(v) \approx & \frac{BM_T(\Lambda + 2\mu)}{\pi b^2} v \\ & \times \left(-\frac{2txy\sqrt{t^2 - a^2 R^2}}{R^4} - a^2 \arctan\left(\frac{2txy\sqrt{t^2 - a^2 R^2}}{R^2(t^2 + a^2 y^2)}\right) \right) \end{aligned}$$

For the same distances and timescales, one expects temperature rises of $O(-3)$ as $v \rightarrow c_t$. These estimates agree well the results derived from the fully coupled problem, and confirms that the thermomechanical heating due to the injection and motion of a dislocation can safely be neglected in comparison with the dissipative heating effect described in Section 2.

5. Conclusions

This article has examined the temperature increase in a crystalline solid resulting from a moving dislocation. Two separate effects have been studied: the dissipative effect associated with the viscous and radiative drag effects, and the thermomechanical temperature rise resulting from the dilatational fields radiated away from the core of edge dislocations.

Simple expressions for the temperature increase associated with the dissipative heating effect have been provided. It has been found that the temperature rise associated with this effect is only considerable for dislocations moving with speeds a significant fraction of the speed of sound, but still insufficient on its own to produce large amounts of localised heating unless large densities of fast moving dislocations are present (cf. Armstrong et al., 1982). The thermomechanical effect has initially been studied both for a coupled thermal and elastodynamic continuum, providing expressions for the temperature field surrounding the core of an injected and moving edge dislocation. The resulting temperature fields have been shown to be very weak, both in terms of the strength of the coupling between the thermal and elastodynamic continua, and in terms of the actual temperature rise. In the coupled problem, asymptotic expressions for the temperature fields have been provided. Based on the weakness of the coupling between the thermal and elastodynamic continua, the uncoupled problem has also been solved, leading to closed-form solutions of the temperature field which may be added to the growing corpus of closed-form solutions of the time-dependent continuum fields of dislocations. In the uncoupled case the magnitude of the thermomechanical effect has also been seen to be small in comparison with the dissipative heating effect.

This study has therefore shown that in the motion of dislocations, the single most important thermal effect is dissipative heating resulting from the overdamped nature of dislocation motion. Effects associated with the presence of dilatational radiation emanating from the core (i.e., thermomechanical heating) may be neglected.

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Appendix

The uncoupled temperature field due to the dilatational fields of the uniformly moving dislocation is

$$\begin{aligned} \theta_{\text{uniform}}(x, y, t) &= \frac{BM_T(3\Lambda + 2\mu)}{\pi b^2} \frac{dy}{2R^4} \\ &\times \left(\frac{\sqrt{d^2 - a^2} R^4 (d(y\sqrt{a^2 - d^2} + dx) - a^2 x)}{y\sqrt{d(d(y^2 - x^2) - 2xy\sqrt{a^2 - d^2}) + a^2 x^2}} \right. \\ &\times \ln\left(\frac{K_1}{K_2}\right) + \frac{\sqrt{d^2 - a^2} R^4 (d(y\sqrt{a^2 - d^2} - dx) + a^2 x)}{y\sqrt{d(2xy\sqrt{a^2 - d^2} + d(y^2 - x^2)) + a^2 x^2}} \\ &\times \ln\left(\frac{K_3}{K_2}\right) - 2\sqrt{t^2 - a^2} R^2 (dR^2 + tx) \Big) \end{aligned} \quad (115)$$

where

$$\begin{aligned} K_1 &= 2y \left(\sqrt{d(-2xy\sqrt{a^2 - d^2} - dx^2 + dy^2) + a^2 x^2 \sqrt{t^2 - a^2} R^2} \right. \\ &\quad \left. + ty\sqrt{d^2 - a^2} - ia^2 R^2 + idtx \right) \end{aligned} \quad (116)$$

$$\begin{aligned} K_2 &= \sqrt{a^2 - d^2} R^4 (d(y\sqrt{a^2 - d^2} + dx) - a^2 x) \\ &\times \sqrt{d(d(y^2 - x^2) - 2xy\sqrt{a^2 - d^2}) + a^2 x^2} \\ &\times (y\sqrt{a^2 - d^2} + dx - t) \end{aligned} \quad (117)$$

$$\begin{aligned} K_3 &= 2iy \left(i\sqrt{d(2xy\sqrt{a^2 - d^2} - dx^2 + dy^2) + a^2 x^2 \sqrt{t^2 - a^2} R^2} \right. \\ &\quad \left. + ity\sqrt{d^2 - a^2} + a^2 x^2 + a^2 y^2 - dtx \right) \end{aligned} \quad (118)$$

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